Computational Approaches in Discovery & Design of Antimicrobial Peptides

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Message from the Guest Editors

Bacterial resistance to antibiotics is still a serious concern worldwide, especially nowadays when dealing with bacterial infections associated with COVID-19. Many computational approaches have been developed to assist in the search and design of antibiotic peptides within the AMPs chemical space. Currently, from classical alignment-based (AB) and alignment-free (AF) prediction algorithms to non-conventional approaches such as complex similarity networks are being applied for AMPs detection. On the other hand, the design and optimization of AMPs are also computationally assisted by the in silico generation of both random and rationally oriented peptide libraries. Artificial-intelligence-inspired evolutionary algorithms and models of sequence evolution have supported the optimization of peptide scaffolds and the rational generation of diversity-oriented libraries, respectively.

This Special Issue of *Antibiotics* invites authors to publish original research including in silico approaches used for the rational search/discovery and design of AMPs. Review papers on this topic are welcome.

Special Issue

Editor-in-Chief

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Message from the Editor-in-Chief

There are very few fields that attract as much attention as scientific endeavor related to antibiotic discovery, use and preservation. The public, patients, scientists, clinicians, policy-makers, NGOs, governments, and supra-governmental organizations are all focusing intensively on it: all are concerned that we use our existing agents more effectively, and develop and evaluate new interventions in time to face emerging challenges for the benefit of present and future generations. We need every discipline to contribute and collaborate: molecular, microbiological, clinical, epidemiological, geographic, economic, social scientific and policy disciples are all key. *Antibiotics* is a nimble, inclusive and rigorous indexed journal as an enabling platform for all who can contribute to solving the greatest broad concerns of the modern world.

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